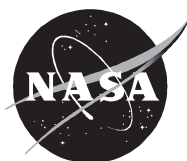# Regularization of the Chapman-Enskog Expansion and Its Description of Shock Structure

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REGULARIZATION OF THE CHAPMAN-ENSKOG EXPANSION AND ITS DESCRIPTION OF SHOCK STRUCTURE*

KUN XU[†]

Abstract. In the continuum transition flow regime, we propose to truncate the Chapman-Enskog expansion of the Boltzmann equation to the Navier-Stokes order only without going to the Burnett or super Burnett orders. However, the local particle collision time has to be generalized to depend not only on the local macroscopic flow variables, but also their gradients in the rarefied gas regime. Based on the gas-kinetic BGK model, the relation between the conventional collision time and the general one is obtained. More specifically, a generalized constitutive relation for stress and heat flux is proposed. This new model is applied to the study of argon gas shock structure. There is good agreement between the predicted shock structure and experimental results for a wide range of Mach numbers.

Key words. Navier-Stokes equations, Chapman-Enskog expansion, continuum transition flow, shock structure

Subject classification. Applied Numerical Mathematics

1. Introduction. It is well recognized that the Navier-Stokes equations of the classical hydrodynamics are incapable of accurately describing shock wave phenomena and also for the flow phenomena in the rarefied regime. In order to improve the Navier-Stokes solutions, much effort has been paid on the construction of higher-order hydrodynamic equations based on the Chapman-Enskog expansion. But the Burnett and super Burnett equations give unstable shock structures in high Mach number cases. For example, no shock structure can be obtained for the Burnett equations after a critical Mach number $M_c = 2.69$ [9]. Even though the argumented Burnett of Zhong et al. and BGK-Burnett equations of Agarwal et al. can significantly improve the Navier-Stokes solutions in the continuum transition regime [7, 14, 1], it is unclear that the stable shock structures of these schemes are coming from the complicated numerical dissipations, such as the use of Steger Warming flux splitting scheme for the inviscid part of the equations [8], or the selected higher-order terms. As analyzed in [10], the failure of the Burnett equations for the shock structure calculation is not too surprising because the applicability of the Chapman-Enskog expansion itself is valid to the small Knudsen numbers. The possible generation of spurious solutions from the higher-order terms in the Chapman-Enskog expansion is another point for criticism [5].

This work is motivated originally by extending the gas-kinetic BGK Navier-Stokes solver to the continuum transition regime [12]. The direct adoption of the Chapman-Enskog expansion with the terms proportional to Knudsen number K_n^2 and K_n^3 in the gas distribution function encounters great difficulty in the shock structure calculations. The critical Mach number for the shock structure based on the BGK-Burnett expansion is found to be around $M_c = 4.5$, and the number becomes even smaller, i.e., $M_c = 2.0$, with the inclusion of super Burnett term [13]. Our numerical experiments show clearly that the successive Chapman-Enskog expansion without selectively choosing higher order terms give divergent results as the Knudsen

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number increases. However, up to the Navier-Stokes order, there is not any limitation on the Mach number for the existence of the stable shock structure. This observation is consistent with the theoretical analysis in [9]. Therefore, it may be possible to truncate the Chapman-Enskog expansion to the Navier-Stokes order only and include the possible non-equilibrium effect on the modification of the viscosity and heat conduction coefficients, the so-called constitutive relations. Traditionally, the particle collision time τ is regarded as a function of macroscopic variables. For example, based on the BGK model [3], we have the collision time $\tau = \mu/p$, where μ is the dynamical viscosity coefficient, such as the Sutherland's law, and p is the pressure. All those viscosity coefficients are basically obtained either experimentally or theoretically in the continuum flow regime [6]. There is no reason to guarantee that this relation is still applicable for the rarefied gas. In this paper, we are going to derive a general particle collision time τ_*, which is applicable in both continuum and continuum transition regime. This derivation is based on the closure of the Chapman-Enskog expansion on the Navier-Stokes order and the BGK equation.

2. Closure of the Chapman-Enskog Expansion. The BGK model in the x-direction can be written as [5]

$$(2.1) \qquad f_t + u f_x = \frac{g - f}{\tau},$$

where f is the gas distribution function and g is the equilibrium state approached by f. Both f and g are functions of space x, time t, particle velocities u, and internal variable ξ. The particle collision time τ determines the viscosity and heat conduction coefficients, i.e., $\mu = \tau p$. The equilibrium state is a Maxwellian distribution,

$$g = \rho \left(\frac{\lambda}{\pi} \right)^{\frac{K+2}{2}} e^{-\lambda((u-U)^2 + \xi_1^2 + \xi_2^2)},$$

where ρ is the density, U is the macroscopic velocity in the x direction, and λ is related to the gas temperature $m/2kT$. For a monatomic gas, ξ_1 and ξ_2 represent the particle velocities in the y and z directions. The relation between mass ρ, momentum ρU, and energy ρE densities with the distribution function f is

$$\begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix} = \int \boldsymbol{\psi} f \, du \, d\xi_1 \, d\xi_2,$$

where $\boldsymbol{\psi}$ has the components

$$\boldsymbol{\psi} = (\psi_1, \psi_2, \psi_3)^T = (1, u, \frac{1}{2}(u^2 + \xi_1^2 + \xi_2^2))^T.$$

Since mass, momentum and energy are conserved during particle collisions, f and g should satisfy the compatibility condition

$$(2.2) \qquad \int (g - f) \psi_\alpha \, du \, d\xi_1 \, d\xi_2 = 0, \qquad \alpha = 1, 2, 3,$$

at any point in space and time.

It is well known that the Euler, the Navier-Stokes, and the Burnett, etc. equations can be derived from the above BGK model using the Chapman-Enskog expansion [6]. The successive expansion of the Chapman-Enskog expansion gives

$$f = g - \tau(g_t + u g_x) + \tau^2(g_{tt} + 2u g_{xt} + u^2 g_{xx}) - \tau^3(g_{ttt} + 3u g_{xtt} + 3u^2 g_{xxt} + u^3 g_{xxx}) + \dots$$

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which corresponds to the Euler (τ^0), the Navier-Stokes (τ), the Burnett (τ^2), and the super Burnett (τ^3) ... orders. With the definition $D = \partial/\partial t + u\partial/\partial x$, we can write the above equation as

$$f = g + \sum_{n=1}^{\infty} (-\tau D)^n g.$$

In the continuum transition regime, the Navier-Stokes equations are expected to be inaccurate and the expansions beyond the Navier-Stokes order have only achieved limited success. As shown by Uribe et al. [10], Bobylev's instability analysis basically provides a range of Knudsen numbers for which the Burnett order is valid [4].

In order to increase the validity of the gas kinetic approach in the continuum transition regime, we have to regularize the Chapman-Enskog expansion. The main idea of this paper is to close the Chapman-Enskog expansion up to the Navier-Stokes order only without going to Burnett or super Burnett orders. But, instead of keeping the original particle collision time τ, we have to construct a general one. In other words, we expand the gas distribution function as

$$(2.3) \qquad\qquad f = g - \tau_*(g_t + ug_x),$$

and τ_* is obtained to have the BGK equation to be satisfied,

$$(2.4) \qquad\qquad f = g - \tau(f_t + uf_x).$$

When the spatial and temporal derivatives of the particle collision times are ignored, from the above two equations (2.3) and (2.4), we can get the relation between the original particle collision time τ and the new one τ_*,

$$(2.5) \qquad\qquad \tau_* = \frac{\tau}{1 + \tau D^2 g/Dg}.$$

Therefore, the local particle collision time depends not only on the macroscopic variables through $\tau = \mu/p$, but also the ratio between the Burnett order $D^2 g$ and the Navier-Stokes order Dg. In the above equation, τ_* depends on the particle velocities, which may introduce great complexity in using its solution. In order to remove the particle velocity dependence in τ_*, we suggest to take a moment on $D^2 g/Dg$ first, such as

$$(2.6) \qquad\qquad \langle \frac{D^2 g}{Dg} \rangle \equiv \int \Psi(u) D^2 g \, du d\xi_1 d\xi_2 \Big/ \int \Psi(u) Dg \, du d\xi_1 d\xi_2.$$

Here we propose to use $\Psi(u) = (u - U)^2$ in the above integration, where U is the local macroscopic velocity. Other choices may be possible. But, due to the fact that both moments of Dg and $D^2 g$ on $(1, u, (1/2)(u^2 + \xi_1^2 + \xi_2^2))$ vanish, the above choice becomes the only one which mimics 'dissipative' energy in some sense. In the expressions of $D^2 g$ and Dg, there exist temporal and spatial derivatives of a Maxwellian. The local spatial derivatives can always be constructed from the interpolated macroscopic flow variables, such as the gradients of mass, momentum, and energy. For the temporal derivatives, they have to be evaluated based on the compatibility conditions, such as $\int D^2 g \psi_\alpha du d\xi_1 d\xi_2 = 0$ and $\int Dg \psi_\alpha du d\xi_1 d\xi_2 = 0$ of the Chapman-Enskog expansion. The detailed numerical procedure is given in [13]. In summary, based on the BGK model and the closure of the Chapman-Enskog expansion on the Navier-Stokes order, we derive a new local particle collision time τ_*, such that

$$(2.7) \qquad\qquad \tau_* = \tau \Big/ \left(1 + \tau \langle D^2 g/Dg \rangle \right).$$

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Based on the above τ_*, the viscosity and heat conduction coefficients will depend on both the macroscopic variables and their slopes. In the continuum regime, since the higher-order dissipation should have less effect than the lower order one, $\langle D^2 g/Dg \rangle$ will theoretically go to zero. This is verified in the following shock structure calculation.

In recent years, an accurate gas-kinetic BGK Navier-Stokes solver (BGK-NS) has been developed for the viscous solution in the continuum regime by the current author and co-workers [12]. In the following argon gas shock structure calculations, we are going to use the above BGK-NS method, but with the implementation of the new particle collision time τ_*. For a monatomic gas modeled by point centers of force, the kinetic theory leads to a viscosity μ proportional to T^s and the Prandtl number $Pr = \mu C_p/\kappa$ is a constant equal to 2/3, where κ is the heat conduction coefficient. The temperature exponent s is given by $s = 1/2 + 2/(v-1)$, where v is the power index of the inter-molecular force law. For argon gas at STP, v= 7.5 is cited by Chapman and Cowling [6] based on early viscosity data. Recent work by Lumpkin and Chapman [7] suggests that v= 9 is a better approximation, which is confirmed through systematic calculation of shock wave profiles. In our calculation, the local Navier-Stokes particle collision time τ is first evaluated according to $\tau = \mu/p$, where $\mu \sim T^s$ and p is the local pressure. Then, the new value τ_* is obtained according to Eq.(2.7). With the general τ_*, the BGK-NS solver is used for the shock structure solution [12]. Since the BGK scheme is a finite volume method, even with intrinsic unit Prandtl number in the BGK model, the heat flux across a cell interface can be modified to simulate a gas with any realistic Prandtl number [12], such as 2/3 for the current argon gas. The shock structure is obtained using a time accurate BGK-NS solver until a steady state is reached. In each calculation with fixed μ and Pr, the mesh size is chosen to make sure that there are at least 30 mesh points in the shock layer and the whole computational domain is covered by 200 grid points.
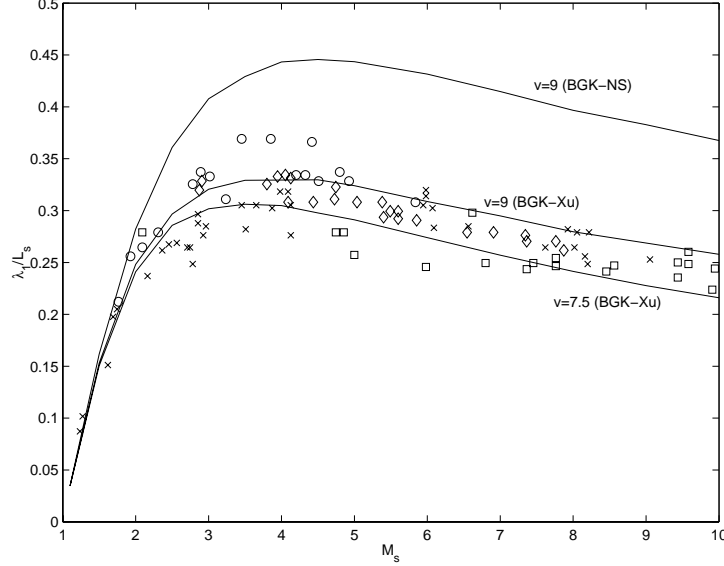

FIG. 2.1. *Comparison of the theoretical shock thickness λ_1/L_s vs. Mach number M_s with the experimental data [2]. The solid lines are the results from the BGK-NS solver [12] and the new BGK-Xu model. The simulations are done for both v= 9.0 and 7.5 cases.*

Studies of the shock structure are generally validated by comparing the reciprocal density thickness with experimental measurements. The thickness is defined as

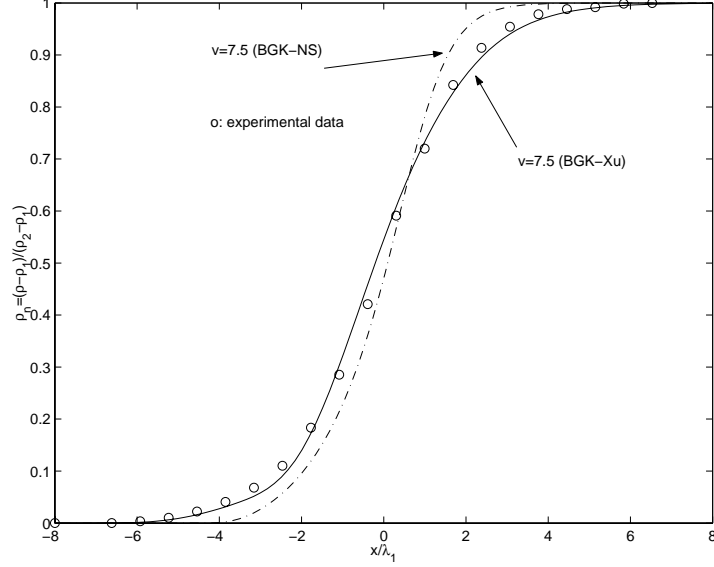$$L_s = (\rho_2 - \rho_1)/(d\rho/dx)_{max}.$$

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FIG. 2.2. *The density $\rho_n = (\rho - \rho_1)/(\rho_2 - \rho_1)$ distribution vs. x/λ_1 inside the shock layer at $M_s = 9$. Dash-dot line, BGK-NS solution with v= 7.5; solid line, BGK-Xu solution with v= 7.5; circles, experimental data for argon gas [2].*

The above shock thickness is normalized by the upstream mean free path,

$$\lambda_1 = \frac{16}{5\sqrt{\pi}} \frac{\mu_1}{\rho_1 \sqrt{2RT_1}}.$$

Figure 2.1 displays the results, where "BGK-NS" refers to the solution of the BGK Navier-Stokes solver with the original particle collision time $\tau = \mu/p$ [12], and "BGK-Xu" refers to the results from the same BGK Navier-Stokes solver but with the implementation of the new value τ_*. Both v= 9 and v= 7.5 cases are tested. All symbols in Figure 2.1 are the experimental data presented in [2], which are extensively used by many others to validate their models [1, 11]. The solution from the current new model (BGK-Xu) matches perfectly with the experimental data. Figure 2.2 presents the density distribution $\rho_n = (\rho - \rho_1)/(\rho_2 - \rho_1)$ vs. x/λ_1, where v= 7.5 is used in both BGK-NS and BGK-Xu solutions. The circles in Figure 2.2 are the experimental data from [2]. From these figures, we can observe that the general particle collision time used significantly improves the results. In the continuum flow regime, where the Mach number of the shock wave goes to 1.0, the BGK-NS and BGK-Xu solutions converge. In other words, τ_* approaches to τ automatically as Knudsen number decreases.

3. Conclusion. In this paper, we have developed a generalized constitutive relation, where the viscosity coefficient depends not only on the macroscopic variables, but also on their gradients. Even with the closure of the Chapman-Enskog expansion on the Navier-Stokes order, the results from this new model agrees well with the experimental data in the study of argon shock structure. The generalization of the collision time from τ to τ_*,

$$\tau_* = \frac{\tau}{1 + \tau \langle D^2 g / Dg \rangle},$$

is important to capture the rarefied gas effect in the continuum transition regime. In the continuum regime, such as the Mach number approaching to 1.0 in the shock case, the contribution from $\langle D^2 g / Dg \rangle$ disappears automatically. This can be understood physically that in the near equilibrium flow the higher order contribution (Burnett $D^2 g$) has much less effect than the lower order term (Navier-Stokes Dg). The further

application of this new BGK-Xu model in the continuum transition regime, such as Couette and Poiseuille flows, will be presented in subsequent papers.

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